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Leges Motus*



Seminar über Fragen der Mechanik

im Rahmen des EFI Projekts



**EMERGING
FIELDS
INITIATIVE**

**Novel Biopolymer Hydrogels
for Understanding
Complex Tissue Biomechanics**

Zu folgendem Vortrag wird herzlich eingeladen

Freitag, **28.06.2019, 14:00 Uhr**, Immerwahrstr. 1, Raum H17

Machine learning in drug development

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An undesirable side effect of drugs are cardiac arrhythmias, in particular a condition called Torsades de Pointes. Current paradigms for drug safety evaluation are costly, lengthy, and conservative, and impede efficient drug development. Here we combine multiscale experiment and simulation, high-performance computing, and machine learning to create an easy-to-use risk assessment diagram to quickly and reliably stratify the pro-arrhythmic potential of new and existing drugs. We capitalize on recent developments in machine learning and integrate information across ten orders of magnitude in space and time to provide a holistic picture of the effects of drugs, either individually or in combination with other drugs. We show, both experimentally and computationally, that drug-induced arrhythmias are dominated by the interplay of two currents with opposing effects: the rapid delayed rectifier potassium current and the L-type calcium current. Using Gaussian process classification, we create a classifier that stratifies safe and arrhythmic domains for any combinations of these two currents. We demonstrate that our classifier correctly identifies the risk categories of 23 common drugs, solely on the basis of their concentrations at 50% current block. Our study shapes the way towards establishing science-based criteria to accelerate drug development, design safer drugs, and reduce heart rhythm disorders.

Prof. Dr.-Ing. P. Steinmann
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